

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032322\
 Data File : BP009521.D
 Acq On : 23 Mar 2022 23:41
 Operator : CG/JU
 Sample : N2031-12 5X
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 CMP-B2-031822-0-2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	5	9	14	rVB	124535	158641	2.74%	0.338%
2	5.393	403	409	433	rBV	1232463	2214668	38.25%	4.719%
3	6.975	666	678	695	rBV	998429	2159358	37.29%	4.601%
4	7.787	809	816	830	rBV	1348283	2378630	41.08%	5.069%
5	8.346	902	911	919	rBV3	97115	330283	5.70%	0.704%
6	8.946	1005	1013	1032	rBV	629024	1365088	23.58%	2.909%
7	10.581	1282	1291	1314	rBV	1573775	3112979	53.76%	6.633%
8	11.999	1525	1532	1534	rBV2	35109	77224	1.33%	0.165%
9	13.051	1704	1711	1723	rBV	1814499	3045015	52.59%	6.489%
10	13.975	1864	1868	1874	rVB4	72325	114417	1.98%	0.244%
11	14.181	1893	1903	1916	rBV2	423076	926685	16.00%	1.975%
12	14.434	1938	1946	1967	rVB	2182117	3817290	65.93%	8.134%
13	15.304	2090	2094	2105	rBV2	42936	77895	1.35%	0.166%
14	15.487	2121	2125	2132	rBV5	41344	85460	1.48%	0.182%
15	15.710	2158	2163	2170	rVB4	45133	79784	1.38%	0.170%
16	15.934	2194	2201	2211	rBV	1176939	2042848	35.28%	4.353%
17	16.175	2236	2242	2255	rBV6	106949	328926	5.68%	0.701%
18	16.316	2261	2266	2273	rBV10	34885	98947	1.71%	0.211%
19	16.416	2279	2283	2290	rVB2	69248	127068	2.19%	0.271%
20	16.551	2302	2306	2311	rVB3	53430	88197	1.52%	0.188%
21	16.798	2344	2348	2353	rVB2	126469	180731	3.12%	0.385%
22	16.969	2374	2377	2381	rVV3	60953	75622	1.31%	0.161%
23	17.022	2382	2386	2394	rVB3	99087	196024	3.39%	0.418%
24	17.192	2409	2415	2421	rBV	2619419	4173264	72.07%	8.893%
25	17.240	2421	2423	2427	rVB	199547	222909	3.85%	0.475%
26	17.781	2512	2515	2521	rBV2	74379	114835	1.98%	0.245%
27	18.069	2560	2564	2568	rBV	272384	407048	7.03%	0.867%
28	18.116	2568	2572	2579	rVB2	387375	697270	12.04%	1.486%
29	18.251	2591	2595	2599	rBV2	384727	655976	11.33%	1.398%
30	18.292	2600	2602	2607	rVB	290764	375747	6.49%	0.801%
31	18.457	2627	2630	2633	rVB2	126217	145935	2.52%	0.311%
32	18.769	2680	2683	2685	rBV2	183688	243116	4.20%	0.518%
33	18.963	2712	2716	2720	rBV	669095	1031413	17.81%	2.198%
34	19.010	2720	2724	2729	rVV4	437095	846720	14.62%	1.804%
35	19.057	2729	2732	2735	rVB2	234528	288414	4.98%	0.615%
36	19.145	2744	2747	2755	rVB2	338019	608361	10.51%	1.296%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.222	2756	2760	2766	rBV	505977	961955	16.61%	2.050%
38	19.375	2783	2786	2791	rVB	263611	357191	6.17%	0.761%
39	19.569	2816	2819	2828	rVV2	636164	1255791	21.69%	2.676%
40	19.651	2830	2833	2839	rVB	483773	766997	13.25%	1.634%
41	19.769	2849	2853	2858	rBV	3229881	4076009	70.39%	8.685%
42	20.351	2949	2952	2956	rBV2	599911	828005	14.30%	1.764%
43	21.310	3110	3115	3120	rBV	3697926	5790236	100.00%	12.338%

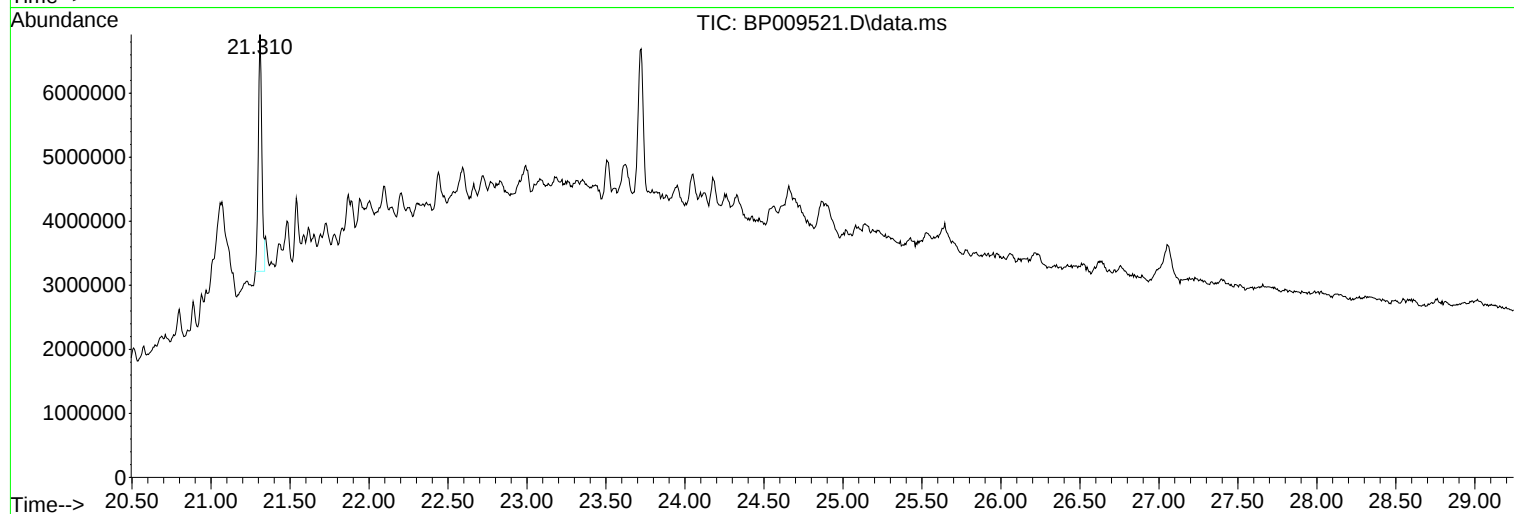
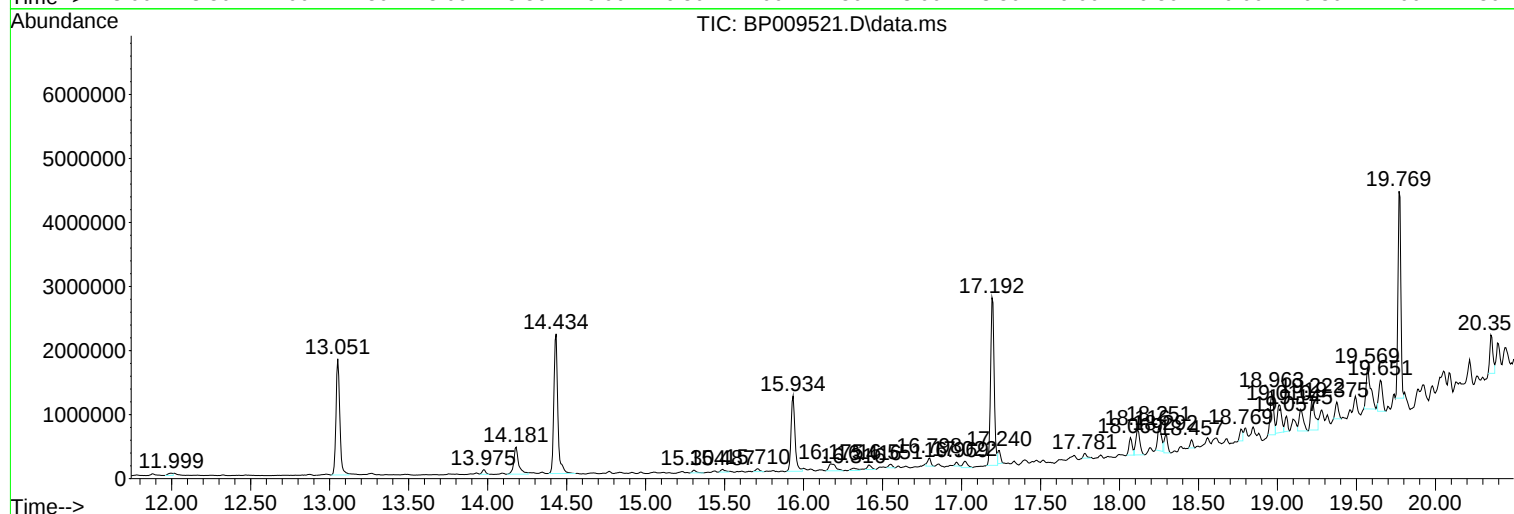
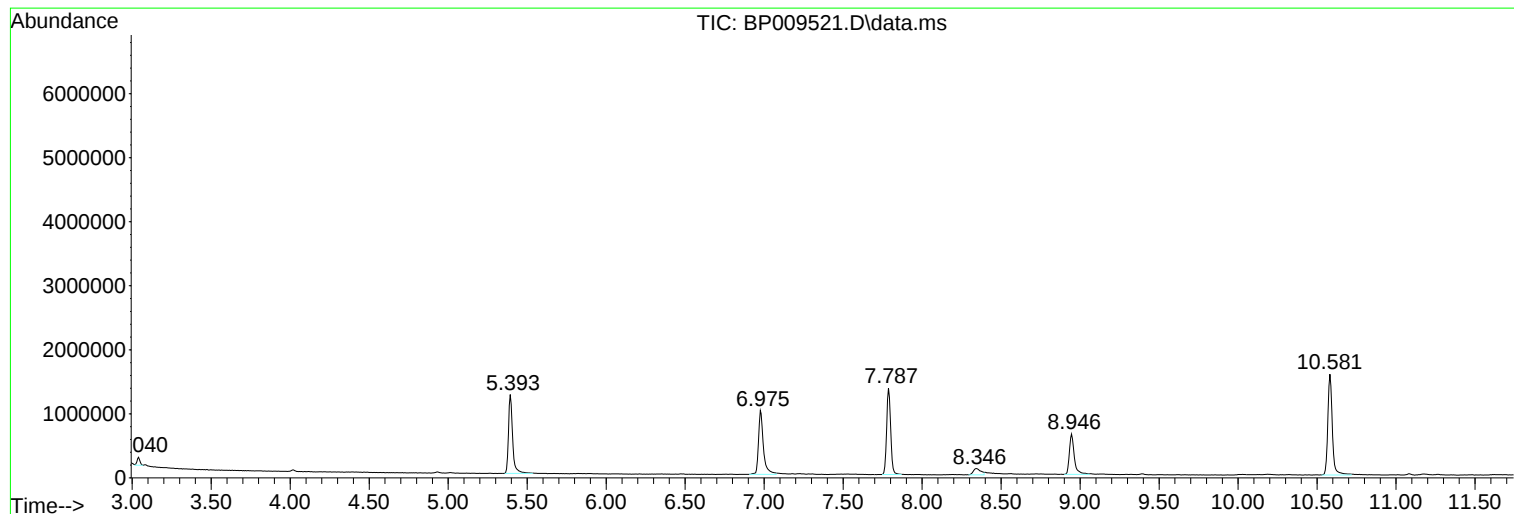
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Misc :
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Instrument :
BNA_P
ClientSampleId :
CMP-B2-031822-0-2

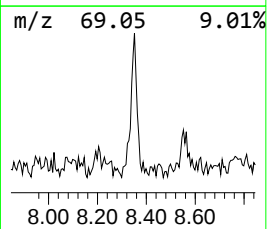
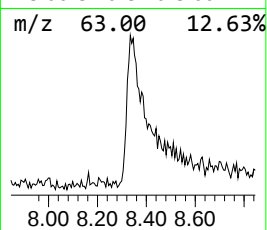
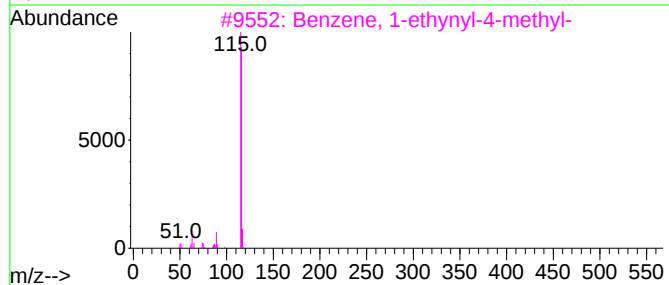
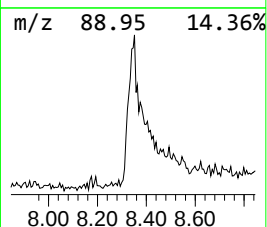
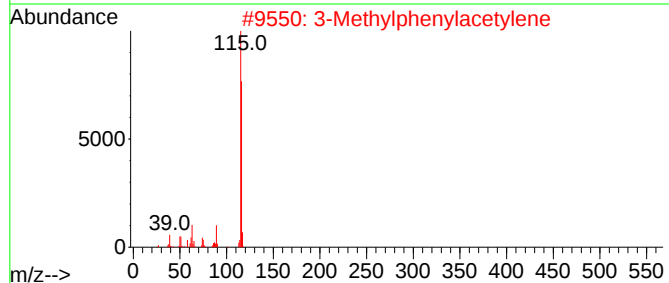
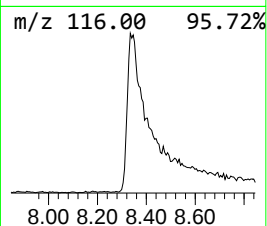
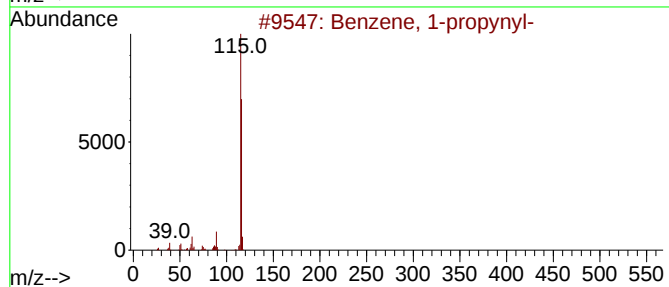
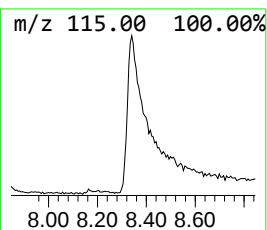
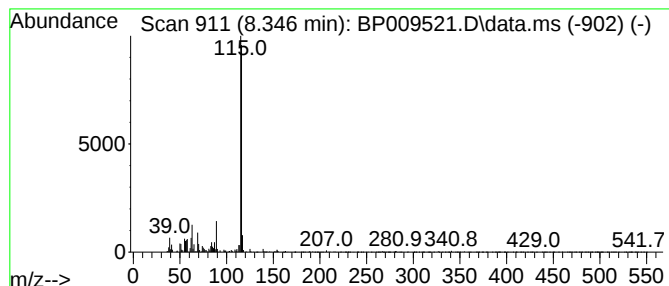
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzene, 1-propynyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.346	2.78 ng	330283	1,4-Dichlorobenzene-d4	7.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-propynyl-	116	C9H8	000673-32-5	90
2			3-Methylphenylacetylene	116	C9H8	000766-82-5	90
3			Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	80
4			Indene	116	C9H8	000095-13-6	76
5			1-indanol trifluoroacetate ester	230	C11H9F3O2	1000376-43-6	72



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Misc :
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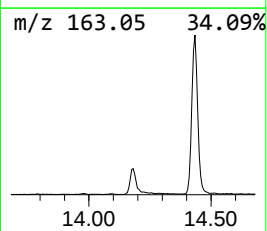
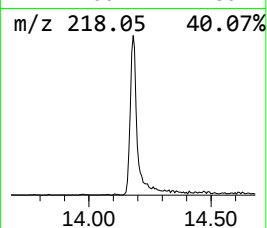
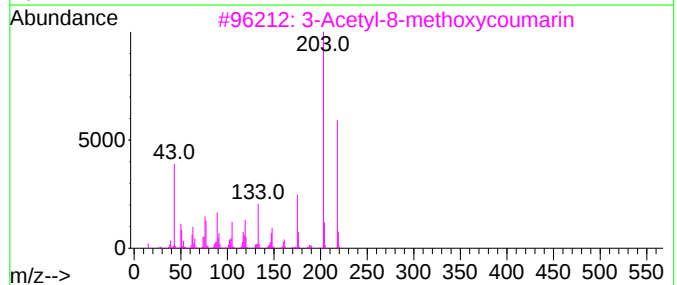
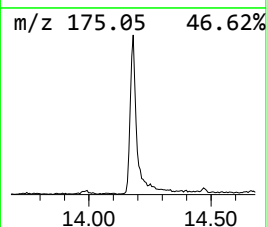
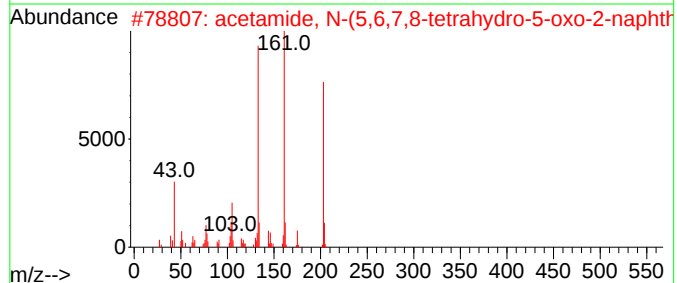
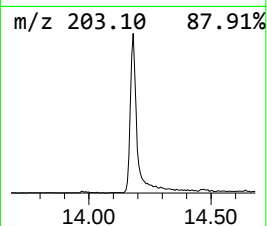
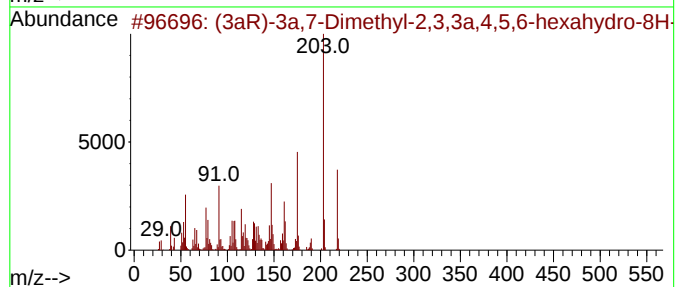
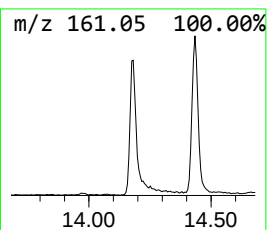
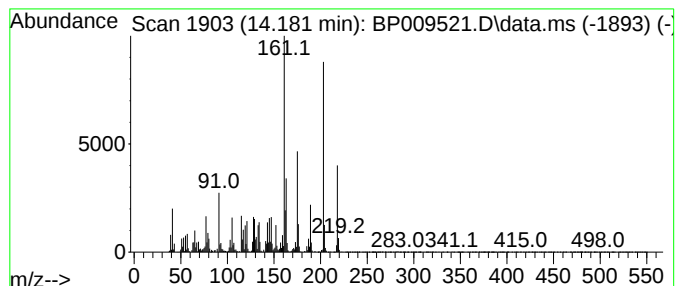
Instrument :
BNA_P
ClientSampleId :
CMP-B2-031822-0-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP031722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (3aR)-3a,7-Dimethyl-2,3,3a,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.181	4.86 ng	926685	Acenaphthene-d10	14.434	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3aR)-3a,7-Dimethyl-2,3,3a,4,5,6...	218	C14H18O2	1000482-61-7	70
2	acetamide, N-(5,6,7,8-tetrahydro...	203	C12H13NO2	1010400-45-2	53
3	3-Acetyl-8-methoxycoumarin	218	C12H10O4	005452-39-1	43
4	2H-[1,2]Dioxeto[3',4':4,5]furo[3...	260	C14H12O5	129833-00-7	41
5	4-n-Butylbenzoic acid, allyl ester	218	C14H18O2	1000293-35-8	38



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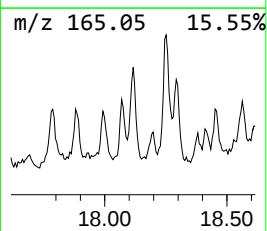
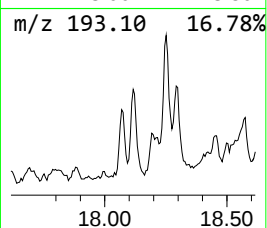
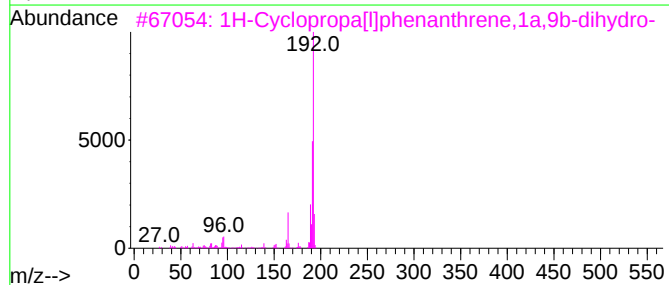
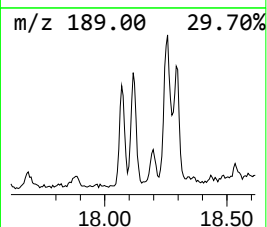
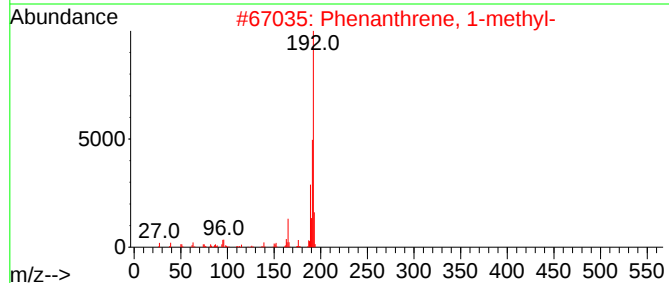
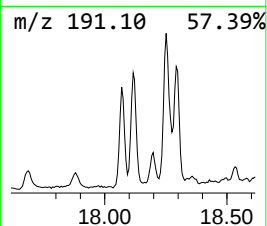
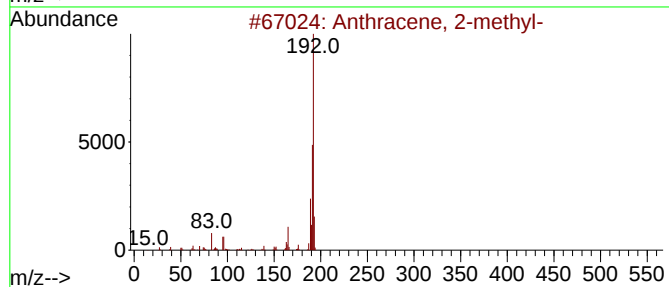
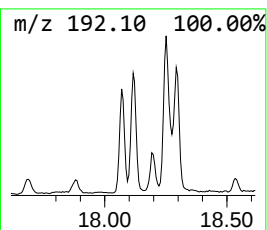
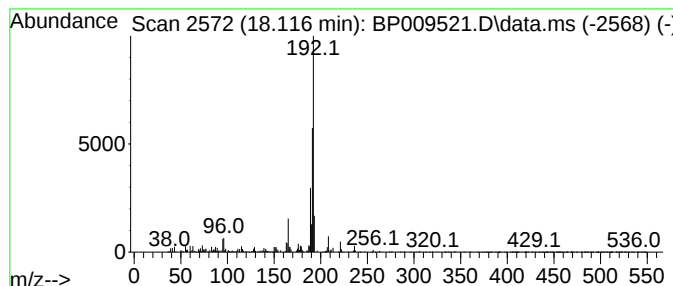
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Anthracene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.116	3.34 ng	697270	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Anthracene, 2-methyl-	192	C15H12	000613-12-7	96
2			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	96
3			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	96
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	96
5			Anthracene, 1-methyl-	192	C15H12	000610-48-0	95



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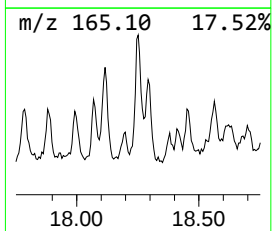
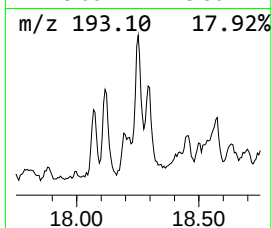
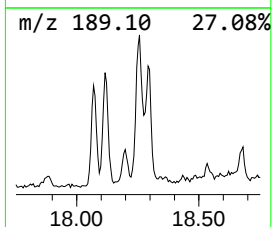
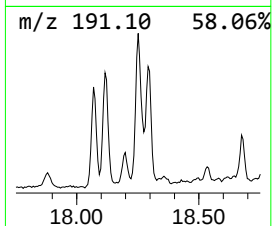
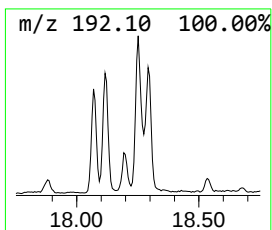
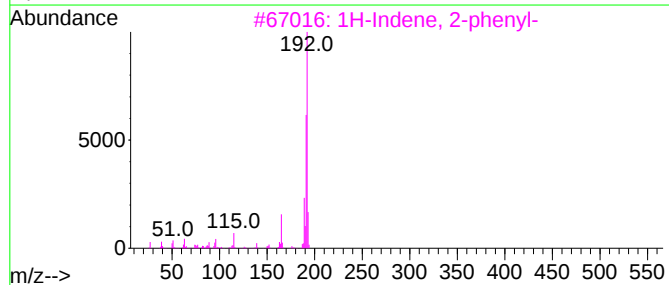
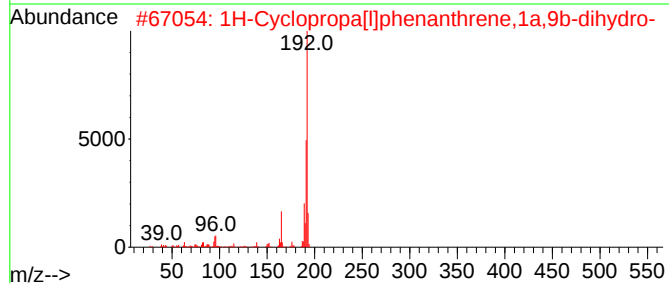
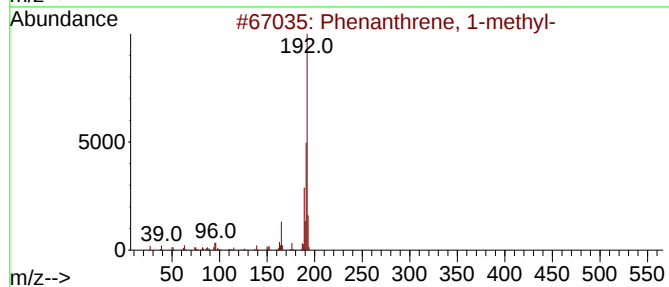
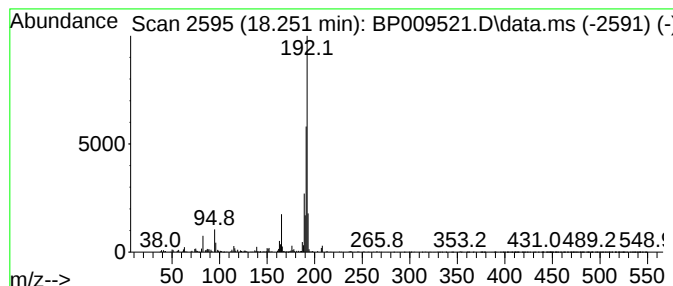
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenanthrene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.251	3.14 ng	655976	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	97
2			1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	96
3			1H-Indene, 2-phenyl-	192	C15H12	004505-48-0	95
4			Anthracene, 1-methyl-	192	C15H12	000610-48-0	95
5			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	95



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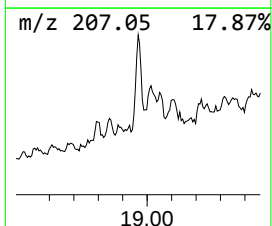
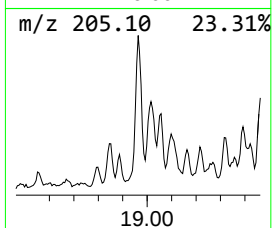
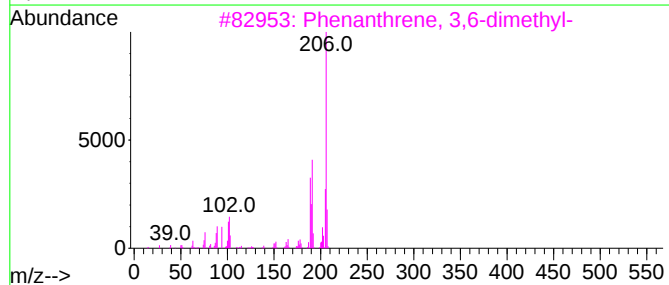
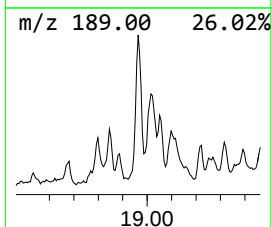
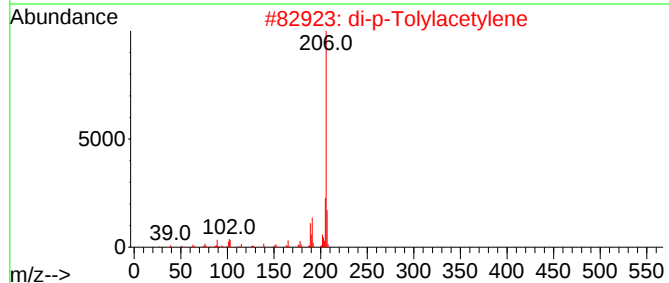
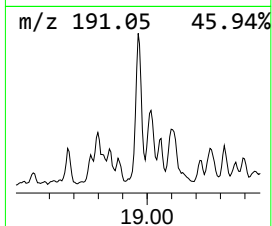
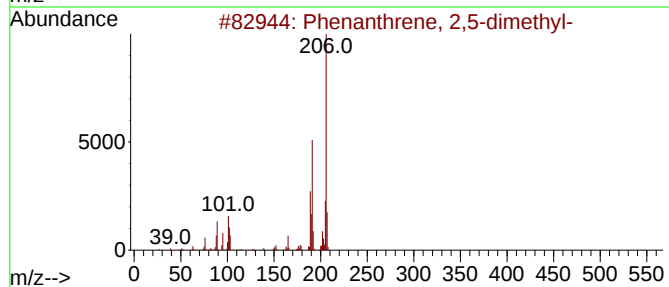
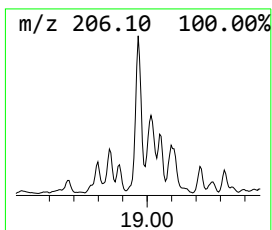
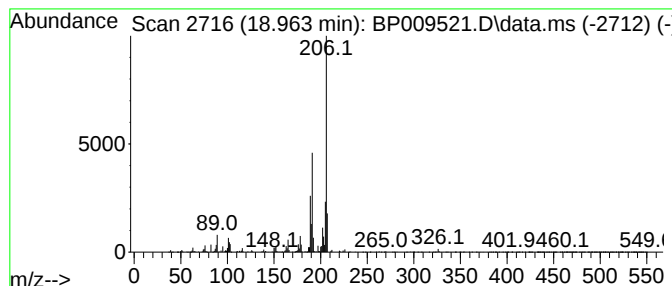
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenanthrene, 2,5-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.963	4.94 ng	1031410	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	94
2			di-p-Tolylacetylene	206	C16H14	002789-88-0	91
3			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90
4			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	90
5			Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032322\
Data File : BP009521.D
Acq On : 23 Mar 2022 23:41
Operator : CG/JU
Sample : N2031-12 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CMP-B2-031822-0-2

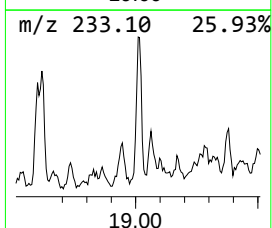
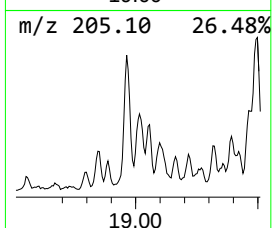
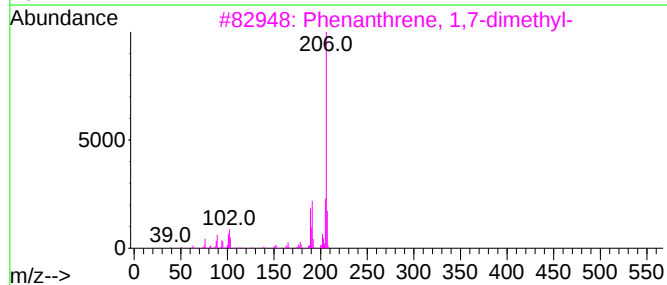
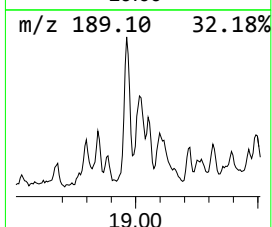
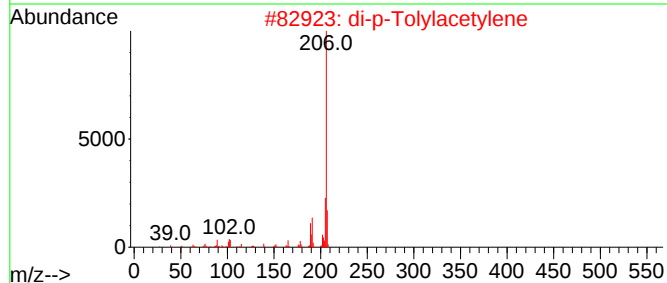
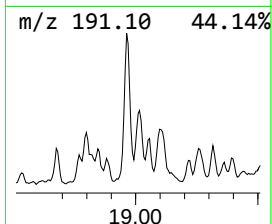
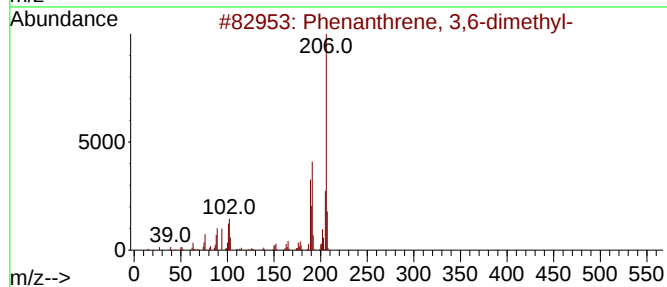
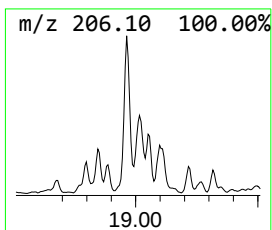
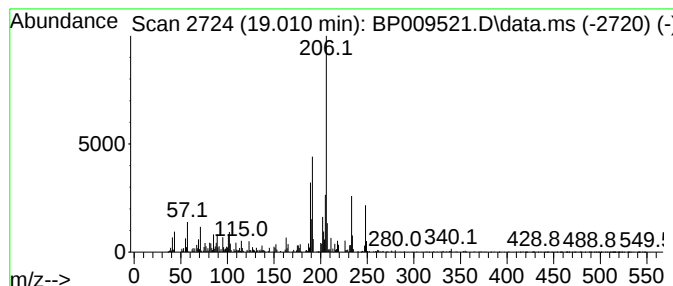
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Phenanthrene, 3,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.010	4.06 ng	846720	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	96
2			di-p-Tolylacetylene	206	C16H14	002789-88-0	89
3			Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	87
4			Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	83
5			1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032322\
Data File : BP009521.D
Acq On : 23 Mar 2022 23:41
Operator : CG/JU
Sample : N2031-12 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CMP-B2-031822-0-2

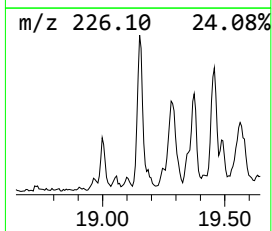
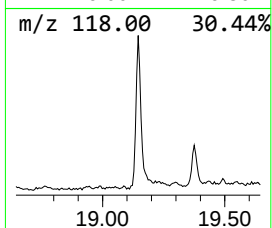
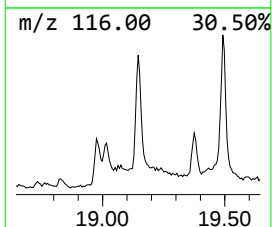
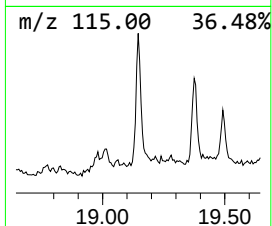
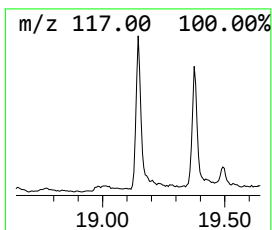
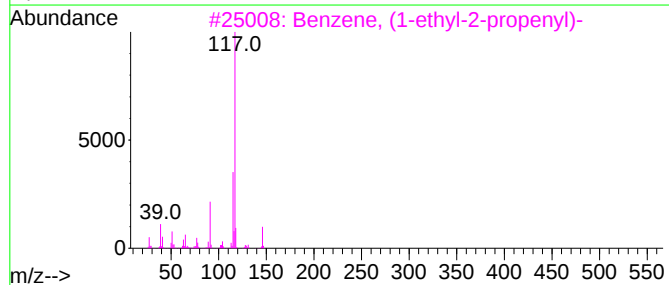
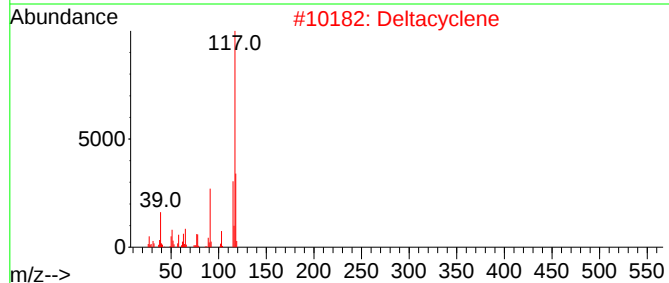
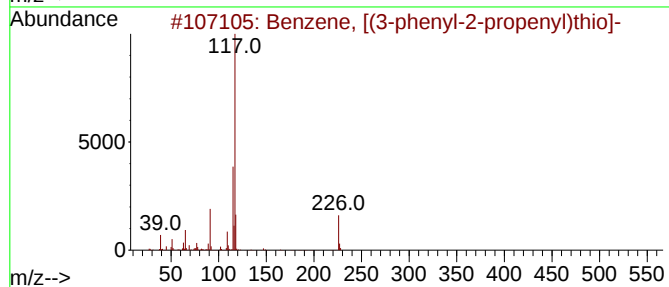
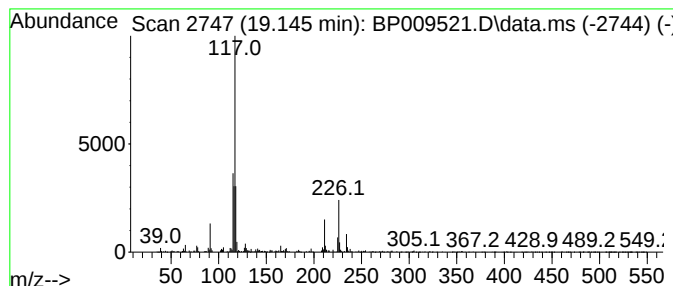
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, [(3-phenyl-2-propenyl)thio]- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.145	2.92 ng	608361	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, [(3-phenyl-2-propenyl)thio]-	226	C15H14S	010276-14-9	59
2			Deltacyclene	118	C9H10	007785-10-6	49
3			Benzene, (1-ethyl-2-propenyl)-	146	C11H14	019947-22-9	47
4			Benzaldehyde, 4-(1-phenyl-2-propenyl)-	238	C16H14O2	1000277-56-1	43
5			1H-Indene, 1-ethyl-2,3-dihydro-	146	C11H14	004830-99-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032322\
Data File : BP009521.D
Acq On : 23 Mar 2022 23:41
Operator : CG/JU
Sample : N2031-12 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CMP-B2-031822-0-2

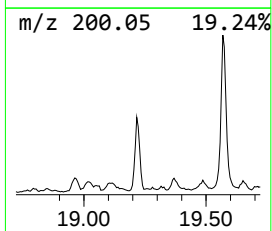
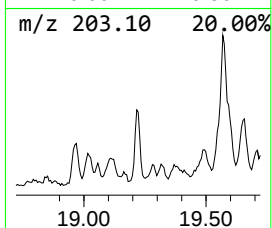
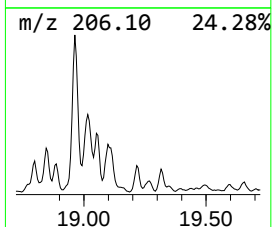
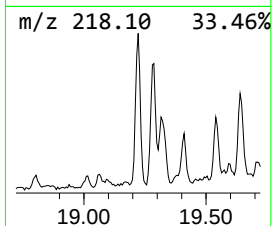
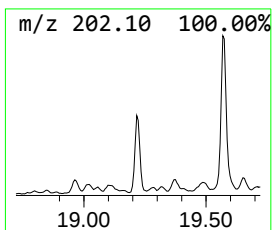
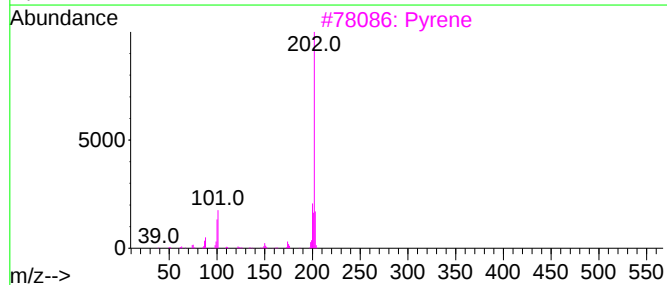
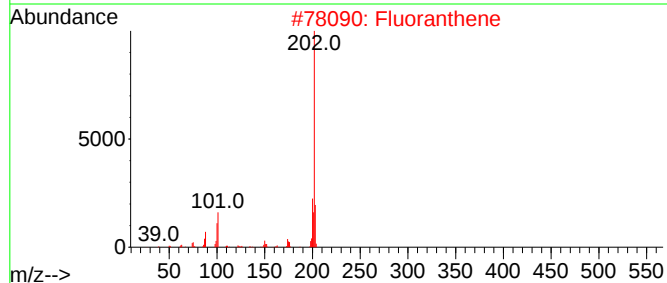
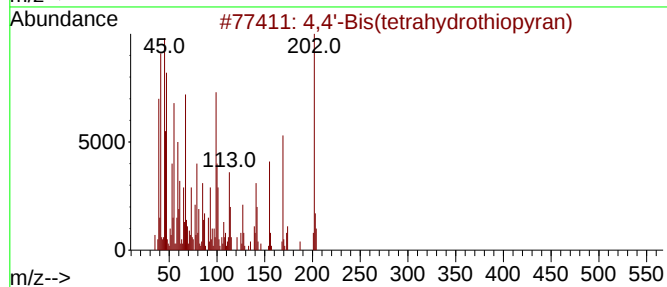
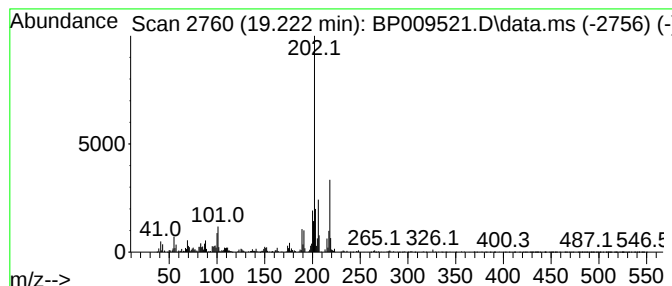
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.222	4.61 ng	961955	Phenanthrene-d10	17.192

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	93
2			Fluoranthene	202	C16H10	000206-44-0	89
3			Pyrene	202	C16H10	000129-00-0	55
4			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	55
5			2-Butenamide, 3-methyl-N-1H-puri...	217	C10H11N5O	021589-34-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032322\
Data File : BP009521.D
Acq On : 23 Mar 2022 23:41
Operator : CG/JU
Sample : N2031-12 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CMP-B2-031822-0-2

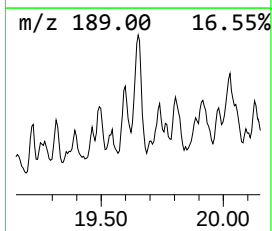
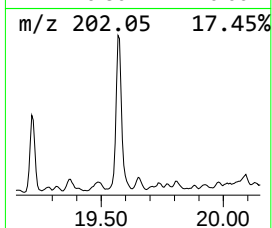
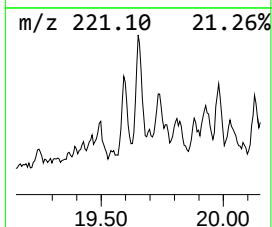
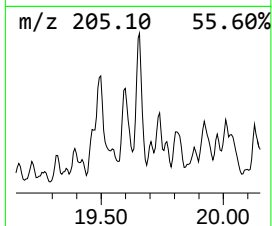
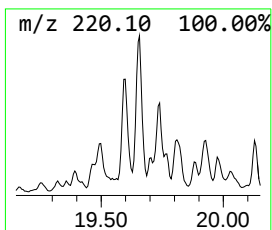
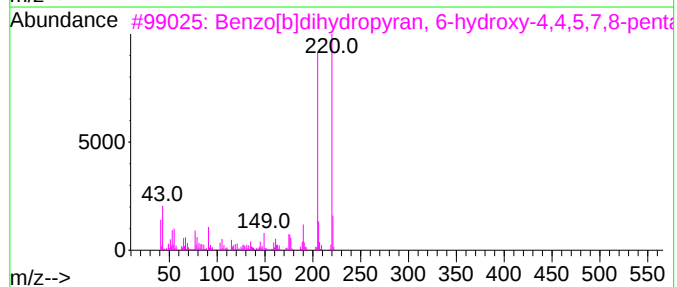
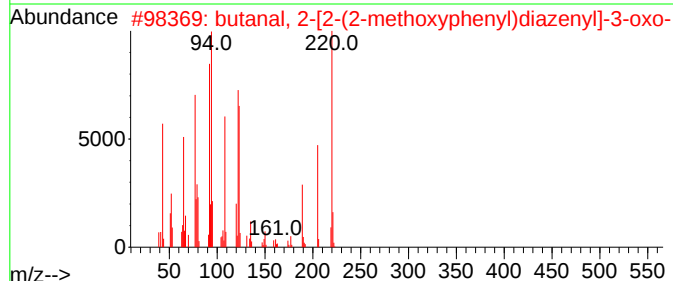
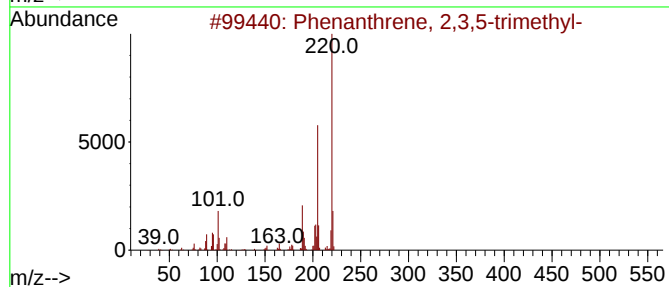
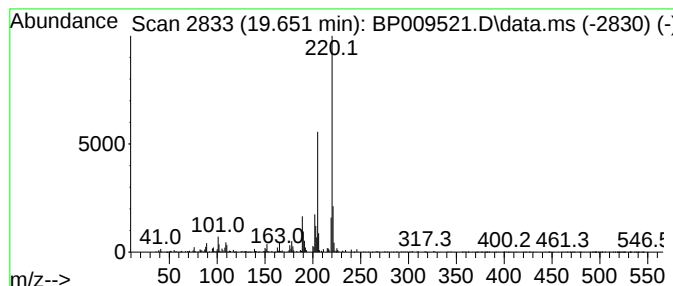
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Phenanthrene, 2,3,5-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.651	2.65 ng	766997	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenanthrene, 2,3,5-trimethyl-	220	C17H16	003674-73-5	91
2			butanal, 2-[2-(2-methoxyphenyl)d...	220	C11H12N2O3	1000396-24-5	64
3			Benzo[b]dihdropyran, 6-hydroxy-...	220	C14H20O2	050442-70-1	59
4			1-(4-Methylphenyl)-4-phenylbuta-...	220	C17H16	037985-11-8	50
5			[4,4'-Bipyrimidine]-2,2',6(1H,1'...	220	C9H8N4O3	018694-06-9	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032322\
Data File : BP009521.D
Acq On : 23 Mar 2022 23:41
Operator : CG/JU
Sample : N2031-12 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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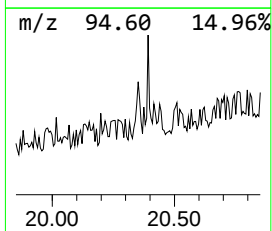
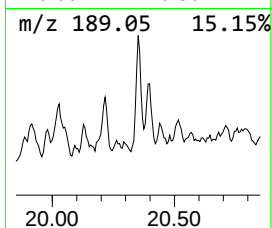
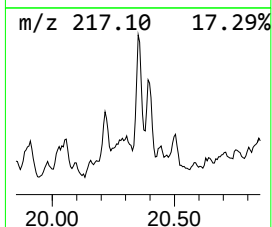
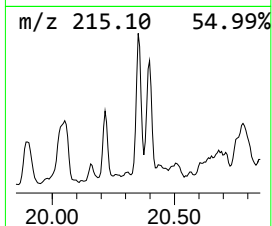
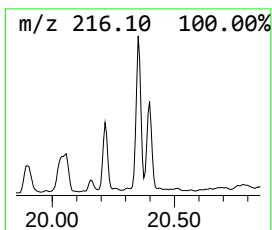
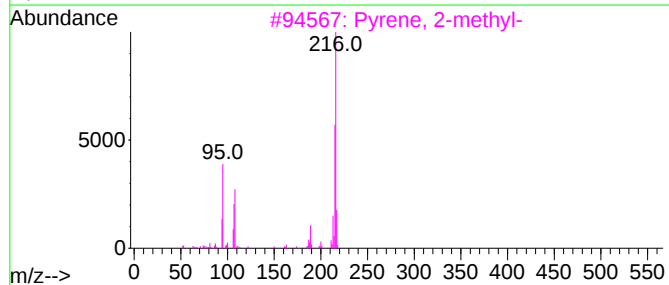
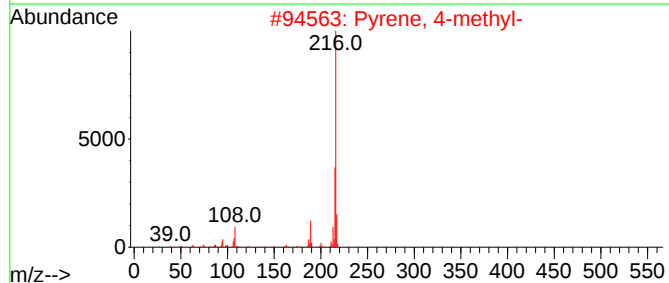
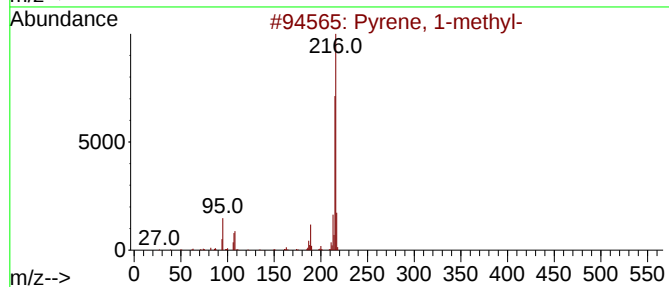
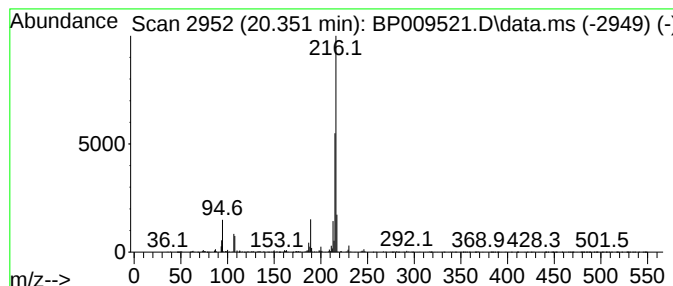
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Pyrene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.351	2.86 ng	828005	Chrysene-d12	21.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyrene, 1-methyl-	216	C17H12	002381-21-7	96
2			Pyrene, 4-methyl-	216	C17H12	003353-12-6	93
3			Pyrene, 2-methyl-	216	C17H12	003442-78-2	87
4			11H-Benzo[a]fluorene	216	C17H12	000238-84-6	87
5			Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP032322\
Data File : BP009521.D
Acq On : 23 Mar 2022 23:41
Operator : CG/JU
Sample : N2031-12 5X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CMP-B2-031822-0-2

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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(3aR)-3a,7-Dime...	14.181	4.9	ng	926685	3	14.434	3817290	20.0
Anthracene, 2-m...	18.116	3.3	ng	697270	4	17.192	4173260	20.0
Phenanthrene, 1...	18.251	3.1	ng	655976	4	17.192	4173260	20.0
Phenanthrene, 2...	18.963	4.9	ng	1031410	4	17.192	4173260	20.0
Phenanthrene, 3...	19.010	4.1	ng	846720	4	17.192	4173260	20.0
Benzene, [(3-ph...	19.145	2.9	ng	608361	4	17.192	4173260	20.0
4,4'-Bis(tetra...	19.222	4.6	ng	961955	4	17.192	4173260	20.0
Phenanthrene, 2...	19.651	2.6	ng	766997	5	21.310	5790240	20.0
Pyrene, 1-methyl-	20.351	2.9	ng	828005	5	21.310	5790240	20.0